



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 11:08 PM UTC

PDB ID : 5F7C / pdb_00005f7c
Title : Crystal structure of Family 31 alpha-glucosidase (BT_0339) from Bacteroides thetaiotaomicron
Authors : Chaudet, M.M.; Rose, D.R.
Deposited on : 2015-12-07
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	FAILED
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

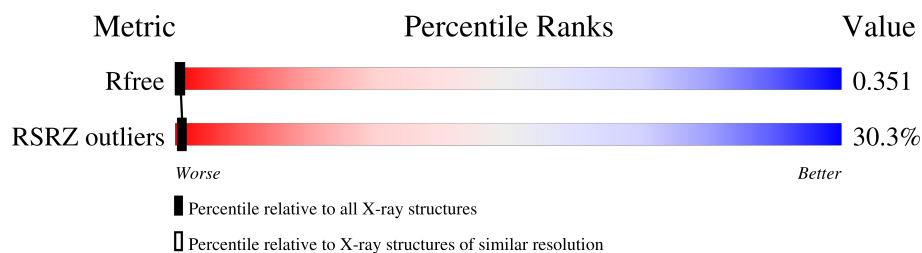
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34019 atoms, of which 14026 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-glucosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	625	Total	C	H	N	O	S	0	0	0
			8422	3229	3426	837	901	29			
1	B	611	Total	C	H	N	O	S	0	0	0
			8403	3150	3512	832	881	28			
1	C	632	Total	C	H	N	O	S	0	0	0
			8637	3278	3548	865	917	29			
1	D	623	Total	C	H	N	O	S	0	0	0
			8490	3185	3540	840	895	30			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	LEU	PHE	conflict	UNP Q8AAX3
A	13	PHE	LEU	conflict	UNP Q8AAX3
A	750	HIS	-	expression tag	UNP Q8AAX3
A	751	HIS	-	expression tag	UNP Q8AAX3
A	752	HIS	-	expression tag	UNP Q8AAX3
A	753	HIS	-	expression tag	UNP Q8AAX3
A	754	HIS	-	expression tag	UNP Q8AAX3
A	755	HIS	-	expression tag	UNP Q8AAX3
A	756	LEU	-	expression tag	UNP Q8AAX3
A	757	ARG	-	expression tag	UNP Q8AAX3
A	758	VAL	-	expression tag	UNP Q8AAX3
A	759	PRO	-	expression tag	UNP Q8AAX3
A	760	ARG	-	expression tag	UNP Q8AAX3
A	761	GLY	-	expression tag	UNP Q8AAX3
A	762	SER	-	expression tag	UNP Q8AAX3
B	12	LEU	PHE	conflict	UNP Q8AAX3
B	13	PHE	LEU	conflict	UNP Q8AAX3
B	750	HIS	-	expression tag	UNP Q8AAX3
B	751	HIS	-	expression tag	UNP Q8AAX3
B	752	HIS	-	expression tag	UNP Q8AAX3
B	753	HIS	-	expression tag	UNP Q8AAX3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	754	HIS	-	expression tag	UNP Q8AAX3
B	755	HIS	-	expression tag	UNP Q8AAX3
B	756	LEU	-	expression tag	UNP Q8AAX3
B	757	ARG	-	expression tag	UNP Q8AAX3
B	758	VAL	-	expression tag	UNP Q8AAX3
B	759	PRO	-	expression tag	UNP Q8AAX3
B	760	ARG	-	expression tag	UNP Q8AAX3
B	761	GLY	-	expression tag	UNP Q8AAX3
B	762	SER	-	expression tag	UNP Q8AAX3
C	12	LEU	PHE	conflict	UNP Q8AAX3
C	13	PHE	LEU	conflict	UNP Q8AAX3
C	750	HIS	-	expression tag	UNP Q8AAX3
C	751	HIS	-	expression tag	UNP Q8AAX3
C	752	HIS	-	expression tag	UNP Q8AAX3
C	753	HIS	-	expression tag	UNP Q8AAX3
C	754	HIS	-	expression tag	UNP Q8AAX3
C	755	HIS	-	expression tag	UNP Q8AAX3
C	756	LEU	-	expression tag	UNP Q8AAX3
C	757	ARG	-	expression tag	UNP Q8AAX3
C	758	VAL	-	expression tag	UNP Q8AAX3
C	759	PRO	-	expression tag	UNP Q8AAX3
C	760	ARG	-	expression tag	UNP Q8AAX3
C	761	GLY	-	expression tag	UNP Q8AAX3
C	762	SER	-	expression tag	UNP Q8AAX3
D	12	LEU	PHE	conflict	UNP Q8AAX3
D	13	PHE	LEU	conflict	UNP Q8AAX3
D	750	HIS	-	expression tag	UNP Q8AAX3
D	751	HIS	-	expression tag	UNP Q8AAX3
D	752	HIS	-	expression tag	UNP Q8AAX3
D	753	HIS	-	expression tag	UNP Q8AAX3
D	754	HIS	-	expression tag	UNP Q8AAX3
D	755	HIS	-	expression tag	UNP Q8AAX3
D	756	LEU	-	expression tag	UNP Q8AAX3
D	757	ARG	-	expression tag	UNP Q8AAX3
D	758	VAL	-	expression tag	UNP Q8AAX3
D	759	PRO	-	expression tag	UNP Q8AAX3
D	760	ARG	-	expression tag	UNP Q8AAX3
D	761	GLY	-	expression tag	UNP Q8AAX3
D	762	SER	-	expression tag	UNP Q8AAX3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total 23	O 23	0	0
2	B	9	Total 9	O 9	0	0
2	C	18	Total 18	O 18	0	0
2	D	17	Total 17	O 17	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.34Å 75.00Å 232.86Å 90.00° 95.14° 90.00°	Depositor
Resolution (Å)	48.81 – 2.60 48.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.81-2.60) 100.0 (48.81-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.302 , 0.349 0.307 , 0.351	Depositor DCC
R_{free} test set	2000 reflections (2.28%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	34019	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	625/761 (82%)	1.30	159 (25%) 1 1	24, 48, 82, 101	0
1	B	611/761 (80%)	1.82	220 (36%) 1 1	51, 69, 92, 104	0
1	C	632/761 (83%)	1.48	193 (30%) 1 1	28, 53, 86, 102	0
1	D	623/761 (81%)	1.55	184 (29%) 1 1	34, 58, 91, 106	0
All	All	2491/3044 (81%)	1.54	756 (30%) 1 1	24, 61, 90, 106	0

All (756) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	ILE	6.7
1	A	470	VAL	6.4
1	D	323	PHE	6.2
1	C	35	TYR	6.2
1	C	54	ASN	5.9
1	D	119	LEU	5.8
1	A	54	ASN	5.7
1	D	115	GLY	5.7
1	D	53	ALA	5.6
1	C	120	PHE	5.6
1	B	356	TRP	5.4
1	B	177	ASP	5.4
1	B	140	TRP	5.3
1	D	328	VAL	5.2
1	B	117	TRP	5.0
1	C	110	VAL	5.0
1	D	54	ASN	5.0
1	C	99	PHE	5.0
1	C	33	ALA	4.9
1	A	720	PRO	4.9
1	C	141	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	141	SER	4.8
1	A	13	PHE	4.8
1	D	601	ILE	4.8
1	D	43	VAL	4.7
1	D	144	LEU	4.7
1	C	53	ALA	4.7
1	B	143	LEU	4.7
1	C	108	LEU	4.7
1	B	141	SER	4.6
1	C	136	ALA	4.6
1	D	137	LEU	4.6
1	B	211	ARG	4.5
1	B	350	GLY	4.5
1	A	40	ASP	4.5
1	B	62	VAL	4.5
1	C	121	THR	4.5
1	C	41	ILE	4.4
1	D	130	ILE	4.4
1	D	143	LEU	4.4
1	B	522	GLY	4.4
1	C	137	LEU	4.4
1	C	428	ALA	4.4
1	C	47	PHE	4.4
1	A	46	PRO	4.3
1	C	113	GLN	4.3
1	C	350	GLY	4.3
1	C	323	PHE	4.3
1	C	356	TRP	4.3
1	B	428	ALA	4.3
1	B	103	ILE	4.3
1	D	718	ILE	4.3
1	B	110	VAL	4.3
1	D	468	ASP	4.3
1	B	136	ALA	4.2
1	D	120	PHE	4.2
1	A	52	LEU	4.2
1	B	323	PHE	4.2
1	D	470	VAL	4.2
1	C	117	TRP	4.2
1	C	40	ASP	4.2
1	C	118	ILE	4.2
1	B	123	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	135	PRO	4.1
1	B	355	ASP	4.1
1	B	68	THR	4.1
1	C	32	THR	4.1
1	C	144	LEU	4.1
1	D	51	LEU	4.1
1	A	368	PRO	4.1
1	B	627	VAL	4.1
1	D	38	ASP	4.1
1	D	24	SER	4.1
1	B	29	CYS	4.1
1	B	333	ASP	4.1
1	D	28	ALA	4.0
1	B	601	ILE	4.0
1	D	589	GLY	4.0
1	D	719	TYR	4.0
1	C	87	GLU	4.0
1	C	470	VAL	4.0
1	A	614	SER	3.9
1	A	686	THR	3.9
1	B	33	ALA	3.9
1	B	118	ILE	3.9
1	B	566	ILE	3.9
1	B	34	VAL	3.9
1	C	106	VAL	3.9
1	D	121	THR	3.9
1	C	473	GLY	3.9
1	C	58	ALA	3.9
1	A	53	ALA	3.8
1	B	667	ASN	3.8
1	A	49	LYS	3.8
1	D	97	LEU	3.8
1	C	45	VAL	3.8
1	C	57	VAL	3.8
1	D	108	LEU	3.8
1	C	70	ILE	3.8
1	A	89	GLU	3.8
1	B	125	THR	3.8
1	C	564	ASN	3.8
1	A	141	SER	3.8
1	C	43	VAL	3.8
1	C	720	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	142	GLU	3.7
1	B	468	ASP	3.7
1	D	326	ASP	3.7
1	B	124	GLY	3.7
1	B	120	PHE	3.7
1	D	113	GLN	3.7
1	A	150	THR	3.7
1	C	713	ASN	3.7
1	B	351	TRP	3.7
1	A	188	GLY	3.7
1	B	186	ARG	3.7
1	D	136	ALA	3.7
1	B	137	LEU	3.6
1	C	143	LEU	3.6
1	C	103	ILE	3.6
1	C	49	LYS	3.6
1	A	140	TRP	3.6
1	B	319	ARG	3.6
1	B	487	TYR	3.6
1	C	367	PHE	3.6
1	A	48	GLN	3.6
1	B	81	LEU	3.6
1	A	70	ILE	3.6
1	B	187	THR	3.6
1	D	71	ILE	3.6
1	D	76	ILE	3.6
1	D	35	TYR	3.6
1	A	42	CYS	3.6
1	A	187	THR	3.6
1	B	454	VAL	3.6
1	C	148	GLN	3.6
1	A	143	LEU	3.6
1	B	52	LEU	3.6
1	D	52	LEU	3.6
1	D	27	LYS	3.6
1	D	60	THR	3.5
1	B	98	GLN	3.5
1	C	125	THR	3.5
1	B	231	GLY	3.5
1	C	476	PRO	3.5
1	D	117	TRP	3.5
1	D	311	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	122	GLN	3.5
1	C	328	VAL	3.5
1	D	324	SER	3.5
1	C	138	ASP	3.5
1	D	65	GLU	3.5
1	D	83	LEU	3.5
1	D	334	ARG	3.5
1	D	118	ILE	3.5
1	B	451	ASP	3.5
1	B	61	ALA	3.5
1	C	619	ILE	3.4
1	A	39	GLY	3.4
1	A	480	ASN	3.4
1	C	115	GLY	3.4
1	D	62	VAL	3.4
1	C	329	ASN	3.4
1	D	438	ALA	3.4
1	B	35	TYR	3.4
1	A	325	ALA	3.4
1	B	135	PRO	3.4
1	D	602	ALA	3.4
1	D	336	ARG	3.4
1	C	34	VAL	3.4
1	C	718	ILE	3.4
1	C	435	TYR	3.4
1	A	721	GLU	3.4
1	A	58	ALA	3.4
1	B	50	GLN	3.4
1	C	42	CYS	3.4
1	C	187	THR	3.3
1	B	108	LEU	3.3
1	C	46	PRO	3.3
1	D	339	HIS	3.3
1	A	131	ASN	3.3
1	D	352	PHE	3.3
1	D	442	TYR	3.3
1	A	477	GLU	3.3
1	D	133	GLU	3.3
1	A	132	VAL	3.3
1	B	27	LYS	3.3
1	C	76	ILE	3.3
1	C	566	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	17	THR	3.3
1	B	439	THR	3.3
1	B	654	TYR	3.3
1	B	720	PRO	3.3
1	C	678	GLU	3.3
1	C	124	GLY	3.3
1	C	337	ALA	3.3
1	A	45	VAL	3.3
1	B	719	TYR	3.3
1	B	438	ALA	3.3
1	D	99	PHE	3.3
1	D	46	PRO	3.2
1	A	473	GLY	3.2
1	A	28	ALA	3.2
1	A	62	VAL	3.2
1	B	57	VAL	3.2
1	B	465	ILE	3.2
1	B	127	ARG	3.2
1	C	56	MET	3.2
1	C	134	GLU	3.2
1	A	324	SER	3.2
1	A	144	LEU	3.2
1	D	140	TRP	3.2
1	A	43	VAL	3.2
1	B	45	VAL	3.2
1	C	158	ASP	3.2
1	B	472	LYS	3.2
1	C	52	LEU	3.2
1	D	32	THR	3.2
1	A	469	ALA	3.2
1	C	130	ILE	3.2
1	D	431	ILE	3.2
1	D	471	TYR	3.2
1	B	694	ARG	3.1
1	B	475	LYS	3.1
1	A	478	LEU	3.1
1	B	51	LEU	3.1
1	A	142	GLU	3.1
1	D	50	GLN	3.1
1	B	508	ALA	3.1
1	C	28	ALA	3.1
1	B	82	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	129	VAL	3.1
1	C	471	TYR	3.1
1	C	55	ASP	3.1
1	D	350	GLY	3.1
1	A	438	ALA	3.1
1	D	360	TRP	3.1
1	B	718	ILE	3.1
1	D	139	ARG	3.1
1	D	96	MET	3.1
1	C	633	LEU	3.1
1	A	600	ALA	3.1
1	A	626	ALA	3.1
1	C	109	SER	3.1
1	D	45	VAL	3.1
1	A	471	TYR	3.1
1	C	322	TYR	3.1
1	B	119	LEU	3.1
1	C	604	LEU	3.1
1	B	436	PRO	3.1
1	C	599	PRO	3.1
1	D	135	PRO	3.1
1	B	116	LYS	3.1
1	B	490	ALA	3.1
1	B	678	GLU	3.0
1	C	336	ARG	3.0
1	A	454	VAL	3.0
1	D	142	GLU	3.0
1	C	107	PRO	3.0
1	C	190	LYS	3.0
1	C	686	THR	3.0
1	A	12	LEU	3.0
1	C	97	LEU	3.0
1	C	119	LEU	3.0
1	D	107	PRO	3.0
1	A	475	LYS	3.0
1	D	116	LYS	3.0
1	A	336	ARG	3.0
1	B	689	ARG	3.0
1	B	469	ALA	3.0
1	C	325	ALA	3.0
1	A	57	VAL	3.0
1	D	129	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	445	LEU	3.0
1	C	51	LEU	3.0
1	C	140	TRP	3.0
1	C	449	LEU	3.0
1	D	37	LYS	3.0
1	C	38	ASP	3.0
1	C	192	ARG	3.0
1	C	457	ILE	3.0
1	A	60	THR	3.0
1	A	136	ALA	3.0
1	B	287	ALA	3.0
1	D	362	PHE	3.0
1	A	20	LEU	2.9
1	B	691	GLN	2.9
1	C	105	ARG	2.9
1	A	130	ILE	2.9
1	B	349	THR	2.9
1	D	349	THR	2.9
1	B	324	SER	2.9
1	B	139	ARG	2.9
1	D	186	ARG	2.9
1	C	168	TYR	2.9
1	D	41	ILE	2.9
1	A	337	ALA	2.9
1	D	34	VAL	2.9
1	A	133	GLU	2.9
1	D	66	GLU	2.9
1	D	704	GLU	2.9
1	C	122	GLN	2.9
1	C	139	ARG	2.9
1	C	186	ARG	2.9
1	D	33	ALA	2.9
1	D	337	ALA	2.9
1	A	690	LEU	2.9
1	B	99	PHE	2.9
1	D	69	LEU	2.9
1	D	109	SER	2.9
1	D	138	ASP	2.9
1	B	453	GLY	2.9
1	D	188	GLY	2.9
1	B	455	THR	2.9
1	B	470	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	25	LEU	2.9
1	D	47	PHE	2.9
1	A	36	GLU	2.8
1	B	26	TRP	2.8
1	C	26	TRP	2.8
1	A	332	CYS	2.8
1	D	42	CYS	2.8
1	D	358	CYS	2.8
1	A	83	LEU	2.8
1	A	439	THR	2.8
1	B	60	THR	2.8
1	B	321	THR	2.8
1	D	351	TRP	2.8
1	D	356	TRP	2.8
1	A	75	ASN	2.8
1	C	86	GLY	2.8
1	B	128	ALA	2.8
1	D	67	TYR	2.8
1	A	323	PHE	2.8
1	A	162	GLU	2.8
1	B	251	GLY	2.8
1	B	59	ASP	2.8
1	D	703	LEU	2.8
1	C	504	VAL	2.8
1	D	57	VAL	2.8
1	A	599	PRO	2.8
1	B	46	PRO	2.8
1	A	601	ILE	2.8
1	C	25	LEU	2.8
1	A	55	ASP	2.8
1	B	328	VAL	2.8
1	C	340	TYR	2.8
1	B	431	ILE	2.7
1	D	103	ILE	2.7
1	B	144	LEU	2.7
1	B	583	SER	2.7
1	B	609	TRP	2.7
1	C	505	TRP	2.7
1	D	466	HIS	2.7
1	D	58	ALA	2.7
1	A	47	PHE	2.7
1	B	433	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	68	THR	2.7
1	B	603	PRO	2.7
1	A	466	HIS	2.7
1	B	521	GLY	2.7
1	C	77	GLY	2.7
1	A	129	VAL	2.7
1	C	132	VAL	2.7
1	D	600	ALA	2.7
1	C	183	PHE	2.7
1	A	351	TRP	2.7
1	B	429	GLY	2.7
1	A	365	GLU	2.7
1	B	671	ARG	2.7
1	D	26	TRP	2.7
1	C	133	GLU	2.7
1	C	142	GLU	2.7
1	D	104	ARG	2.7
1	B	715	VAL	2.7
1	A	38	ASP	2.7
1	D	176	TYR	2.7
1	B	345	ILE	2.7
1	A	689	ARG	2.7
1	D	124	GLY	2.7
1	C	111	GLU	2.7
1	D	329	ASN	2.7
1	B	185	LYS	2.7
1	B	344	VAL	2.7
1	B	592	LYS	2.7
1	C	62	VAL	2.7
1	C	150	THR	2.7
1	C	185	LYS	2.7
1	B	476	PRO	2.7
1	D	31	PRO	2.7
1	B	448	GLN	2.6
1	B	42	CYS	2.6
1	B	446	LEU	2.6
1	C	188	GLY	2.6
1	C	447	LYS	2.6
1	D	190	LYS	2.6
1	C	596	TRP	2.6
1	D	564	ASN	2.6
1	B	53	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	167	ALA	2.6
1	B	157	PRO	2.6
1	D	147	PRO	2.6
1	A	326	ASP	2.6
1	A	139	ARG	2.6
1	B	261	LYS	2.6
1	B	43	VAL	2.6
1	A	135	PRO	2.6
1	B	337	ALA	2.6
1	B	567	VAL	2.6
1	D	100	SER	2.6
1	B	121	THR	2.6
1	C	79	THR	2.6
1	C	50	GLN	2.6
1	B	38	ASP	2.6
1	A	719	TYR	2.6
1	C	88	TYR	2.6
1	D	81	LEU	2.6
1	A	458	LYS	2.6
1	B	669	GLU	2.6
1	C	36	GLU	2.6
1	C	39	GLY	2.6
1	A	31	PRO	2.6
1	A	428	ALA	2.6
1	C	438	ALA	2.6
1	D	476	PRO	2.6
1	A	360	TRP	2.6
1	B	25	LEU	2.6
1	B	295	LEU	2.6
1	B	442	TYR	2.6
1	C	156	TYR	2.6
1	D	322	TYR	2.6
1	C	27	LYS	2.6
1	B	111	GLU	2.6
1	B	133	GLU	2.6
1	A	560	PRO	2.6
1	B	325	ALA	2.6
1	D	461	PHE	2.6
1	C	691	GLN	2.6
1	D	48	GLN	2.6
1	D	55	ASP	2.5
1	D	331	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	310	LEU	2.5
1	B	690	LEU	2.5
1	B	129	VAL	2.5
1	B	232	VAL	2.5
1	A	448	GLN	2.5
1	B	193	ALA	2.5
1	B	602	ALA	2.5
1	D	325	ALA	2.5
1	A	713	ASN	2.5
1	A	26	TRP	2.5
1	A	355	ASP	2.5
1	C	431	ILE	2.5
1	A	51	LEU	2.5
1	A	446	LEU	2.5
1	A	598	TYR	2.5
1	B	688	GLU	2.5
1	B	473	GLY	2.5
1	D	183	PHE	2.5
1	D	44	THR	2.5
1	B	695	TRP	2.5
1	A	460	ASP	2.5
1	B	161	ARG	2.5
1	C	59	ASP	2.5
1	C	355	ASP	2.5
1	B	36	GLU	2.5
1	C	162	GLU	2.5
1	A	521	GLY	2.5
1	C	715	VAL	2.5
1	A	352	PHE	2.5
1	C	82	PHE	2.5
1	B	591	ASN	2.5
1	A	172	SER	2.5
1	B	486	LEU	2.5
1	C	72	ARG	2.5
1	A	692	GLY	2.5
1	B	340	TYR	2.5
1	D	148	GLN	2.5
1	D	344	VAL	2.5
1	B	49	LYS	2.4
1	A	434	THR	2.4
1	B	449	LEU	2.4
1	D	357	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	196	SER	2.4
1	C	466	HIS	2.4
1	A	191	GLU	2.4
1	B	114	GLY	2.4
1	B	664	PRO	2.4
1	C	147	PRO	2.4
1	B	709	TYR	2.4
1	D	660	PHE	2.4
1	C	104	ARG	2.4
1	A	564	ASN	2.4
1	C	123	ASP	2.4
1	C	608	TRP	2.4
1	D	529	ASP	2.4
1	A	341	PRO	2.4
1	D	39	GLY	2.4
1	A	185	LYS	2.4
1	A	328	VAL	2.4
1	A	571	VAL	2.4
1	B	322	TYR	2.4
1	D	132	VAL	2.4
1	B	58	ALA	2.4
1	B	104	ARG	2.4
1	B	336	ARG	2.4
1	C	61	ALA	2.4
1	C	64	ARG	2.4
1	C	166	ALA	2.4
1	A	71	ILE	2.4
1	A	181	ILE	2.4
1	B	71	ILE	2.4
1	C	224	LEU	2.4
1	C	24	SER	2.4
1	A	158	ASP	2.4
1	B	497	GLU	2.4
1	C	31	PRO	2.4
1	D	114	GLY	2.4
1	D	488	GLN	2.4
1	D	571	VAL	2.4
1	A	340	TYR	2.4
1	B	562	PHE	2.4
1	C	287	ALA	2.4
1	C	719	TYR	2.4
1	D	105	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	347	LEU	2.4
1	A	445	LEU	2.4
1	C	357	LEU	2.4
1	A	455	THR	2.4
1	A	149	GLU	2.4
1	C	653	GLU	2.4
1	B	570	ASP	2.4
1	A	189	LYS	2.4
1	C	472	LYS	2.4
1	C	436	PRO	2.4
1	D	720	PRO	2.4
1	D	630	GLY	2.4
1	C	48	GLN	2.4
1	B	298	TYR	2.3
1	B	471	TYR	2.3
1	D	435	TYR	2.3
1	D	479	LEU	2.3
1	B	331	ILE	2.3
1	B	150	THR	2.3
1	B	434	THR	2.3
1	C	339	HIS	2.3
1	A	66	GLU	2.3
1	C	712	GLU	2.3
1	A	190	LYS	2.3
1	B	260	SER	2.3
1	B	268	SER	2.3
1	D	49	LYS	2.3
1	A	596	TRP	2.3
1	C	29	CYS	2.3
1	C	63	PRO	2.3
1	C	159	GLY	2.3
1	B	223	PHE	2.3
1	D	193	ALA	2.3
1	A	431	ILE	2.3
1	B	41	ILE	2.3
1	B	712	GLU	2.3
1	D	134	GLU	2.3
1	D	162	GLU	2.3
1	D	40	ASP	2.3
1	B	311	TRP	2.3
1	B	595	PRO	2.3
1	C	360	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	77	GLY	2.3
1	D	98	GLN	2.3
1	D	665	VAL	2.3
1	A	25	LEU	2.3
1	B	83	LEU	2.3
1	D	310	LEU	2.3
1	B	76	ILE	2.3
1	A	35	TYR	2.3
1	B	79	THR	2.3
1	B	447	LYS	2.3
1	C	112	LYS	2.3
1	B	480	ASN	2.3
1	B	564	ASN	2.3
1	B	316	TRP	2.3
1	D	122	GLN	2.3
1	D	441	TRP	2.3
1	C	429	GLY	2.3
1	A	723	VAL	2.3
1	A	137	LEU	2.3
1	D	625	LEU	2.3
1	A	33	ALA	2.3
1	B	509	ALA	2.3
1	C	182	ALA	2.3
1	D	566	ILE	2.3
1	A	56	MET	2.3
1	B	474	MET	2.3
1	A	436	PRO	2.3
1	B	109	SER	2.3
1	B	668	SER	2.3
1	B	711	ARG	2.3
1	C	127	ARG	2.3
1	C	687	GLY	2.3
1	B	665	VAL	2.3
1	D	106	VAL	2.3
1	D	171	PHE	2.3
1	D	345	ILE	2.2
1	B	56	MET	2.2
1	C	126	LYS	2.2
1	C	89	GLU	2.2
1	C	569	GLU	2.2
1	D	598	TYR	2.2
1	C	102	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	174	PRO	2.2
1	B	659	ASP	2.2
1	C	128	ALA	2.2
1	C	163	ILE	2.2
1	D	506	ALA	2.2
1	A	125	THR	2.2
1	A	134	GLU	2.2
1	C	44	THR	2.2
1	B	516	TYR	2.2
1	B	598	TYR	2.2
1	D	340	TYR	2.2
1	A	329	ASN	2.2
1	A	227	GLN	2.2
1	A	691	GLN	2.2
1	A	24	SER	2.2
1	B	496	LYS	2.2
1	C	475	LYS	2.2
1	A	562	PHE	2.2
1	B	313	PHE	2.2
1	B	556	PHE	2.2
1	B	584	HIS	2.2
1	A	364	GLU	2.2
1	C	60	THR	2.2
1	C	590	THR	2.2
1	D	187	THR	2.2
1	C	507	ARG	2.2
1	A	322	TYR	2.2
1	C	176	TYR	2.2
1	B	155	LEU	2.2
1	B	271	SER	2.2
1	B	281	LEU	2.2
1	B	552	ASP	2.2
1	C	146	ASP	2.2
1	C	451	ASP	2.2
1	C	478	LEU	2.2
1	D	153	ILE	2.2
1	D	597	HIS	2.2
1	B	330	GLU	2.2
1	A	161	ARG	2.2
1	A	670	ASN	2.2
1	D	717	PRO	2.2
1	A	361	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	30	LYS	2.2
1	B	485	LEU	2.2
1	C	114	GLY	2.2
1	D	449	LEU	2.2
1	D	661	LEU	2.2
1	D	333	ASP	2.2
1	A	331	ILE	2.2
1	D	465	ILE	2.2
1	B	47	PHE	2.2
1	A	61	ALA	2.1
1	D	61	ALA	2.1
1	D	332	CYS	2.1
1	B	63	PRO	2.1
1	C	560	PRO	2.1
1	D	436	PRO	2.1
1	C	74	TYR	2.1
1	C	116	LYS	2.1
1	C	606	LYS	2.1
1	C	474	MET	2.1
1	C	690	LEU	2.1
1	C	703	LEU	2.1
1	D	446	LEU	2.1
1	C	589	GLY	2.1
1	A	339	HIS	2.1
1	D	277	ASP	2.1
1	D	584	HIS	2.1
1	A	15	PHE	2.1
1	A	433	PHE	2.1
1	B	28	ALA	2.1
1	D	166	ALA	2.1
1	A	712	GLU	2.1
1	B	65	GLU	2.1
1	B	134	GLU	2.1
1	D	596	TRP	2.1
1	A	186	ARG	2.1
1	B	296	ARG	2.1
1	C	694	ARG	2.1
1	D	711	ARG	2.1
1	B	32	THR	2.1
1	D	455	THR	2.1
1	D	590	THR	2.1
1	B	147	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	185	LYS	2.1
1	B	238	TYR	2.1
1	A	451	ASP	2.1
1	B	619	ILE	2.1
1	C	465	ILE	2.1
1	C	601	ILE	2.1
1	B	507	ARG	2.1
1	C	681	TRP	2.1
1	D	558	THR	2.1
1	A	126	LYS	2.1
1	A	437	LYS	2.1
1	B	458	LYS	2.1
1	D	173	PRO	2.1
1	B	625	LEU	2.1
1	B	106	VAL	2.1
1	A	685	PHE	2.1
1	C	65	GLU	2.1
1	D	36	GLU	2.1
1	B	190	LYS	2.1
1	A	44	THR	2.1
1	B	677	PRO	2.1
1	D	145	PRO	2.1
1	A	50	GLN	2.1
1	B	220	GLN	2.1
1	A	604	LEU	2.1
1	A	633	LEU	2.1
1	D	462	GLY	2.1
1	C	587	TYR	2.1
1	A	72	ARG	2.0
1	C	468	ASP	2.0
1	C	149	GLU	2.0
1	B	172	SER	2.0
1	D	218	SER	2.0
1	B	112	LYS	2.0
1	B	624	LYS	2.0
1	A	356	TRP	2.0
1	B	194	THR	2.0
1	B	237	THR	2.0
1	C	81	LEU	2.0
1	D	347	LEU	2.0
1	D	445	LEU	2.0
1	D	486	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	363	ASN	2.0
1	B	178	GLY	2.0
1	D	616	ILE	2.0
1	A	665	VAL	2.0
1	C	613	TYR	2.0
1	A	64	ARG	2.0
1	B	548	PHE	2.0
1	C	161	ARG	2.0
1	A	472	LYS	2.0
1	C	324	SER	2.0
1	A	63	PRO	2.0
1	B	264	LEU	2.0
1	B	680	GLN	2.0
1	D	559	LEU	2.0
1	A	77	GLY	2.0
1	A	561	ASN	2.0
1	A	718	ILE	2.0
1	B	153	ILE	2.0
1	B	542	GLY	2.0
1	B	102	ARG	2.0
1	C	366	ARG	2.0

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

There are no ligands in this entry.

5.5 Other polymers ⓘ

There are no such residues in this entry.